Sparse Supernodal Solver exploiting Low-Rankness Property

Grégoire Pichon, Eric Darve, Mathieu Faverge, Pierre Ramet, Jean Roman

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September 6th, 2017 - Sparse Days

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Introduction

Current sparse direct solver for 3D problems

- $\Theta(n^2)$ time complexity
- $\Theta(n^{\frac{4}{3}})$ memory complexity
- BLAS 3 operations

Block Low-Rank solver

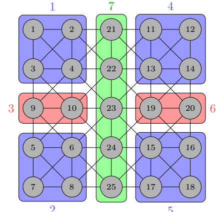
- Large blocks are compressed into a low-rank form
- Operations keep untouched the global behaviour of PaStiX
- *Minimal Memory* strategy allows to save memory
- *Just-In-Time* strategy allows to reduce time-to-solution

Objective: build an algebraic low-rank solver following the supernodal approach of PaStiX, with block-data structures

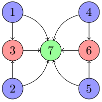
Symbolic Factorization

General approach

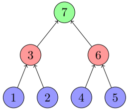
1. Build a partition with the nested dissection process
2. Compress information on data blocks
3. Compute the block elimination tree using the block quotient graph



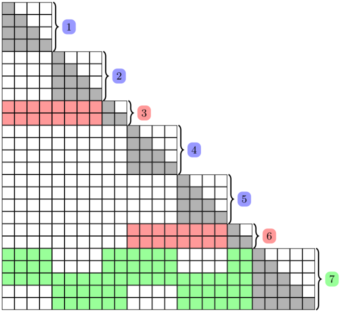
Adjacency graph (G).



Quotient graph (G^*/P) $= (G/P)^*$



Elimination tree (T).

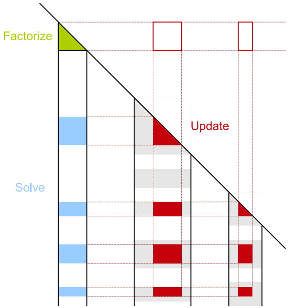


Factorized matrix (L).

Numerical Factorization

Algorithm to eliminate the column block k

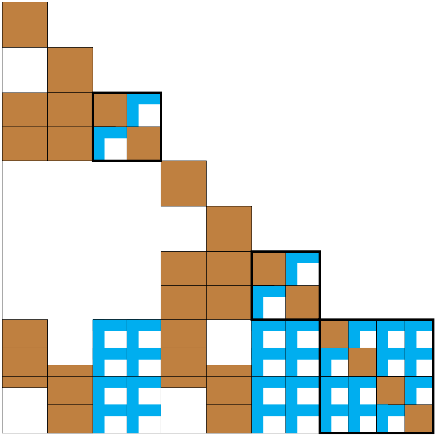
1. Factorize the diagonal block (POTRF/GETRF)
2. Solve off-diagonal blocks in the current column (TRSM)
3. Update the trailing matrix with the column's contribution (GEMM)



Parallelism

- Right-Looking
- Left-Looking

Block-Low-Rank Compression – Symbolic Factorization



Large off-diagonal are low-rank, in the form uv^t

Some Related Works

Block Low-Rank solvers

- BLR-MUMPS introduced an approach focused on reducing the time to solution which is close to our *Just-In-Time* strategy
- LSTC developed compression/recompression techniques in a dense context

Other approaches for sparse

- Strumpack HSS by Ghysels et al. utilizes randomized sampling to perform an efficient extend-add
- HODLR by Darve et al. uses pre-selection of rows and columns (BDLR)
- $\mathcal{H}$-LU by Hackbusch et al. does not fully exploit the symbolic factorization

Block-Low-Rank Algorithm

Approach

- Large supernodes are partitioned into a set of smaller supernodes
- Large off-diagonal blocks are represented as low-rank blocks

Operations

- Diagonal blocks are dense
- TRSM are performed on low-rank off-diagonal blocks
- GEMM are performed between low-rank off-diagonal blocks. It creates contributions to dense or low-rank blocks: this is the extend-add problem

Compression techniques

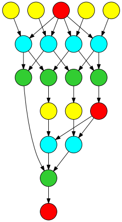
- SVD, RRQR for now
- Possible extension to any algebraic method: ACA, randomized techniques...

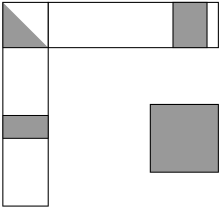
Strategy *Just-In-Time*

Compress L

1. Eliminate each column block
   - **1.1** Factorize the dense diagonal block
     Compress off-diagonal blocks belonging to the supernode
   - **1.2** Apply a TRSM on LR blocks (cheaper)
   - **1.3** LR update on dense matrices (*LR2GE* extend-add)
2. Solve triangular systems with low-rank blocks

	Compression
	GETRF (Facto)
	TRSM (Solve)
	LR2LR (Update)
	LR2GE (Update)





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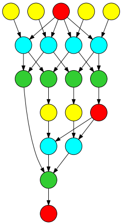

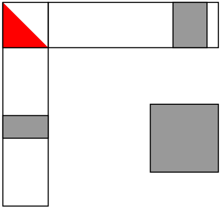

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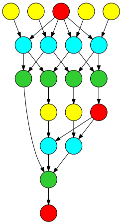

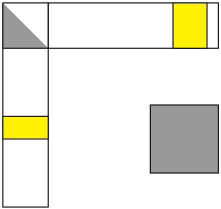

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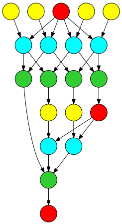

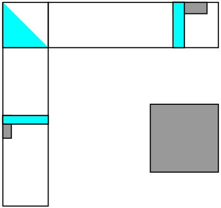

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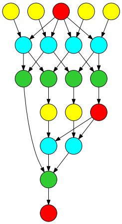

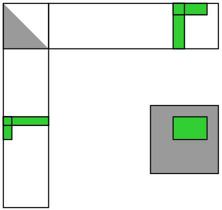

Strategy *Minimal Memory*

Compress A

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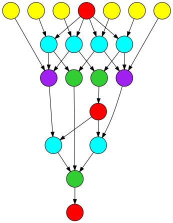

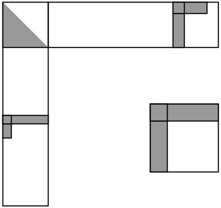

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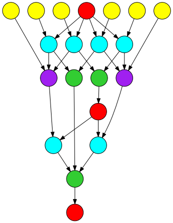

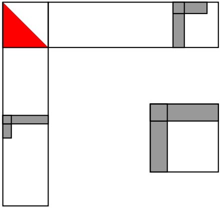

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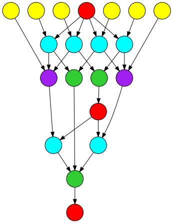

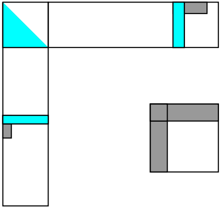

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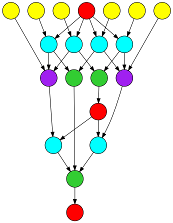
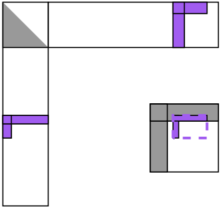




Comparison of both strategies

Memory consumption

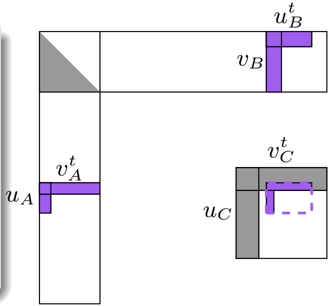
- *Minimal Memory* strategy really saves memory
- *Just-In-Time* strategy reduces the size of L' factors, but supernodes are allocated dense at the beginning: no gain in pure *right-looking*

Low-Rank extend-add

- *Minimal Memory* strategy requires expensive extend-add algorithms to update (recompress) low-rank structures with the *LR2LR* kernel
- *Just-In-Time* strategy continues to apply dense update at a smaller cost through the *LR2GE* kernel

Focus on the *LR2LR* kernel

- Update of C with contribution from blocs A and B
- The low-rank matrix $u_{AB}v_{AB}^t$ is added to $u_C v_C^t$
- $u_{AB}v_{AB}^t = (u_A(v_A^t v_B))u_B^t$ or $u_{AB}v_{AB}^t = u_A((v_A^t v_B)u_B^t)$
- Eventually, recompression of $(v_A^t v_B)$



LR2LR kernel using SVD

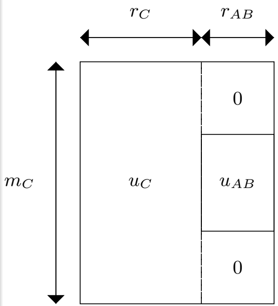
A low-rank structure $u_C v_C^t$ receives a low-rank contribution $u_{AB} v_{AB}^t$.

Algorithm

$$A = u_C v_C^t + u_{AB} v_{AB}^t = \left([u_C, u_{AB}]\right) \times \left([v_C, v_{AB}]\right)^t$$

- QR: $[u_C, u_{AB}] = Q_1 R_1$ $\Theta(m(r_C + r_{AB})^2)$
- QR: $[v_C, v_{AB}] = Q_2 R_2$ $\Theta(n(r_C + r_{AB})^2)$
- SVD: $R_1 R_2^t = u \sigma v^T$ $\Theta((r_C + r_{AB})^3)$

$$A = (Q_1 u \sigma) \times (Q_2 v)^t$$



Optimizations using RRQR to reduce complexity to $\Theta(n(r_C + r_{AB}) r_C^*)$

Experimental setup

Machine: 2 INTEL Xeon $E5-2680v3$ at 2.50 GHz

- 128 GB
- 24 threads

3D Matrices from The SuiteSparse Matrix Collection

- *Audi*: structural problem ($943\ 695$ dofs)
- *Atmosmodj*: atmospheric model ($1\ 270\ 432$ dofs)
- *Geo1438*: geomechanical model of earth ($1\ 437\ 960$ dofs)
- *Hook*: model of a steel hook ($1\ 498\ 023$ dofs)
- *Serena*: gas reservoir simulation ($1\ 391\ 349$ dofs)
- + Laplacian: Poisson problem (7-points stencil)

Parallelism is obtained following PASTIX static scheduling for multi-threaded architectures

Parameters

Entry parameters

- Tolerance τ: absolute parameter (normalized for each block)
- Compression method: SVD or RRQR
- Compression strategy: *Minimal Memory* or *Just-In-Time*
- Blocking sizes: between 128 and 256 in following experiments

Strategy *Minimal Memory*

- Blocks are compressed at the beginning
- Each contribution implies a recompression

Strategy *Just-In-Time*

- Blocks are compressed just before a supernode is eliminated
- Those blocks are never uncompressed

Costs distribution on the Atmosmodj matrix with $\tau = 10^{-8}$

	Dense	*Just-In-Time*		*Minimal Memory*	
		RRQR	SVD	RRQR	SVD
Factorization time (s)					
Compression	-	49.53	418.5	15.20	180.9
Block factorization (GETRF)	0.9635	1.000	1.003	1.074	1.104
Panel solve (TRSM)	15.80	6.970	6.526	11.16	6.946
Update					
LR product	-	64.10	91.15	193.1	94.36
LR addition	-	-	-	774.6	6523
Dense udpate (GEMM)	418.7	47.94	47.03	-	-
Total	*436*	*169*	*564*	*995*	*6806*
Solve time (s)	2.43	1.54	1.8	2.22	1.29
Factors final size (GB)	15.9	7.4	6.86	11.4	6.76
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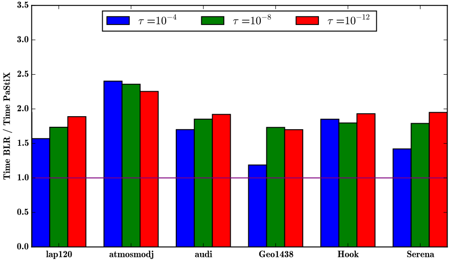
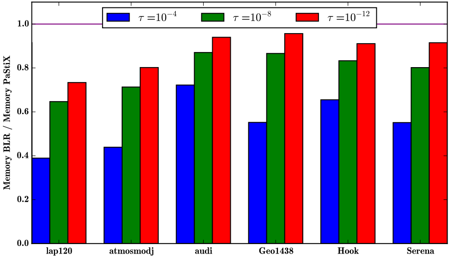
Behaviour of RRQR/*Minimal Memory*

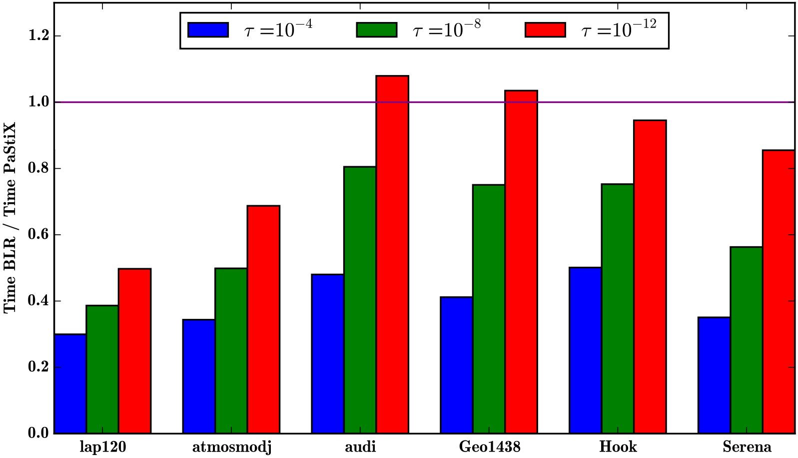


Performance

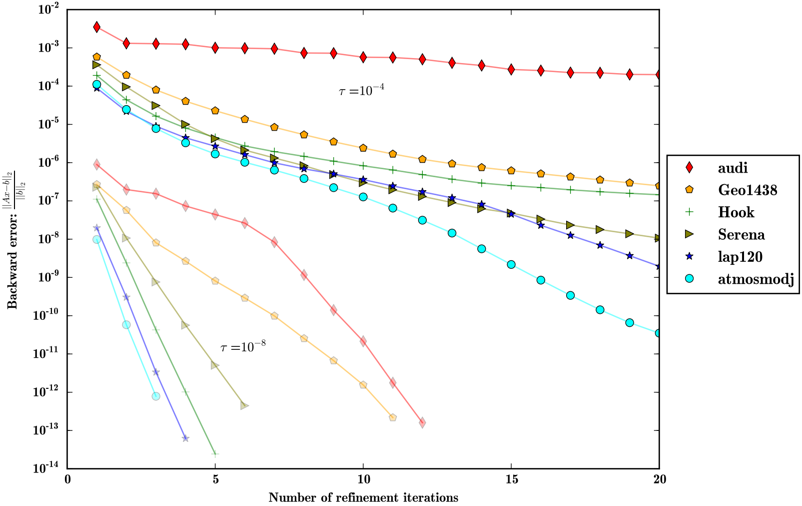


Memory footprint

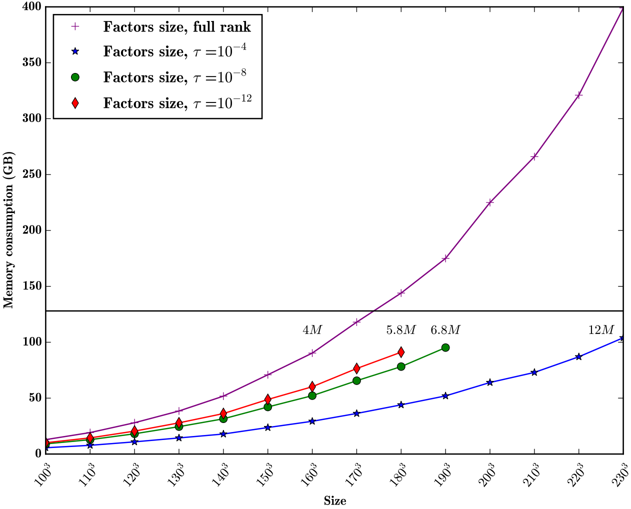
Performance of RRQR/*Just-In-Time*



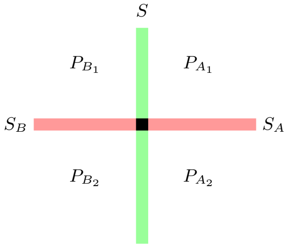
Convergence of RRQR/*Minimal Memory*

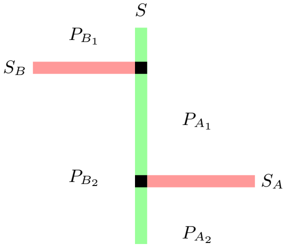


Scaling on Laplacians: Memory Consumption RRQR/*Minimal Memory*



Ongoing work with E. Esnard and M. Predari

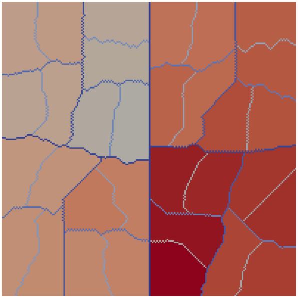




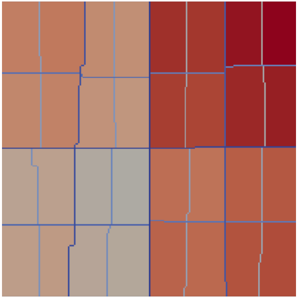
- Single interaction between S and $S_A \cup S_B$ in the original graph
- Two large interaction blocks $P_{A_1} \cup P_{B_1}$ and $P_{A_2} \cup P_{B_2}$ during the factorization

- Double interaction: between S and S_A and between S and S_B in the original graph
- Three "large" interaction blocks during the factorization

Example on a 200^2 Laplacian



Scotch ordering



Aligned ordering

Conclusion

Block Low-Rank solver

- Allows to see how to use the symbolic structure and the extend-add issues in a supernodal context
- The version presented follows the parallelism of PASTIX
- On-going work to implement efficiently this approach over the PARSEC runtime system

Ordering strategies

- Study of a nested dissection designed to increase compressibility
- Add pre-selection to isolate data which is not compressible, and thus reduce the overhead of trying to compress uncompressible blocks

PaStiX 6.0.0alpha is now available!

http://gitlab.inria.fr/solverstack/pastix

- Support shared memory with different schedulers:
  - sequential
  - static scheduler
  - PaRSEC runtime system
- Low-rank support
- Cholesky and LU factorizations

Thank you.